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REFERENCE: Short Term Scientific Mission, COST CM0601
Beneficiary: Diogo Fialho de Almeida, New University of Lisbon (PT)
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SCIENTIFIC REPORT

PURPOSE OF VISIT

Energy deposition models at the molecular level for biological systems are needed in some biomedical applications of radiation. In these models, processes leading to ionic fragmentation of molecules play an important role. To understand the dynamics of these processes electron scattering experiments in which primary electrons, recoil ions and secondary electron are detected in coincidence should be carried out to describe them in term of the corresponding cross section. In this project we propose the measurement of ionic fragmentation cross section of biomolecules (THF, THFA and DNA bases) by electron impact as well as the energy and spatial distribution of secondary electron generated in these processes.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

The initial proposed objectives were:

- Setting up the experiment for fragment ion detection in coincidence with secondary electron: TOF calibration, electronic adjustments;
- Measurement of the partial ionization cross section of THF and THFA by electron impact from threshold to 1500 eV;
- Electron impact ionization cross section for DNA bases;
- Energy and angular distribution of secondary electron produced by ionizing collisions.

During the stage of my scientific mission to CSIC, most of the work has been devoted to set-up an experiment for obtaining electron energy loss spectra on a sample of biological relevant molecules, in this particular case THF. The EEL is monitored on a hemispherical energy analyzer. The experimental apparatus is formed of two constituent parts: a) the first area is the electron gun and collision chamber, b) the second area is mainly comprised of a 180º hemispherical analyzer. The first area (see Fig. 1 below) contains a simple electron gun formed by a filament with a Pierce geometry element, followed by an extractor and integrator electrodes. Between these electrodes there is a pair of deflecting plates for each x and y axis. After these elements there's a chamber where the collision between the electrons and the target molecule take place, followed by a small chamber fitted with a focusing lens system. The second area of the apparatus begins with a second pair of deflecting plates, followed by an Einzel lens system and the entrance to the hemispherical analyzer itself. Electron detection is done via a channeltron detector mounted on the exit of the hemispherical analyzer (see figure below).

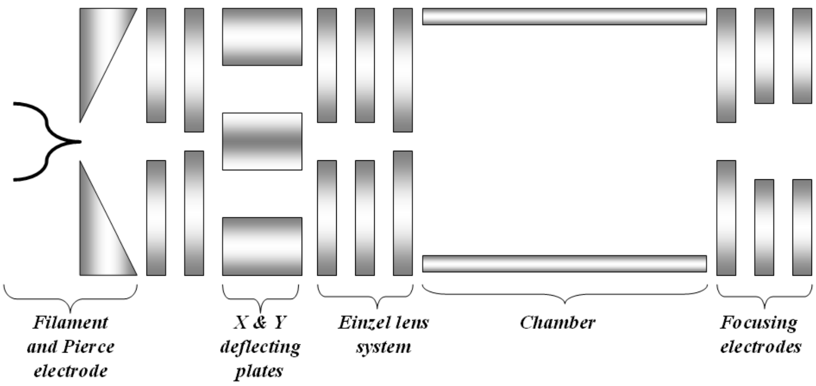


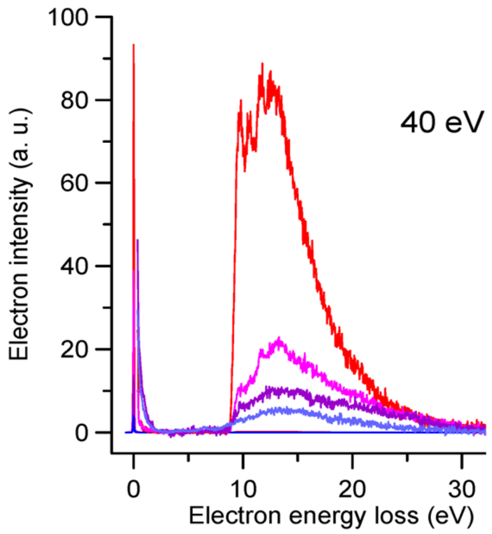
Fig. 1: Schematic representation of the electron gun and collision system.

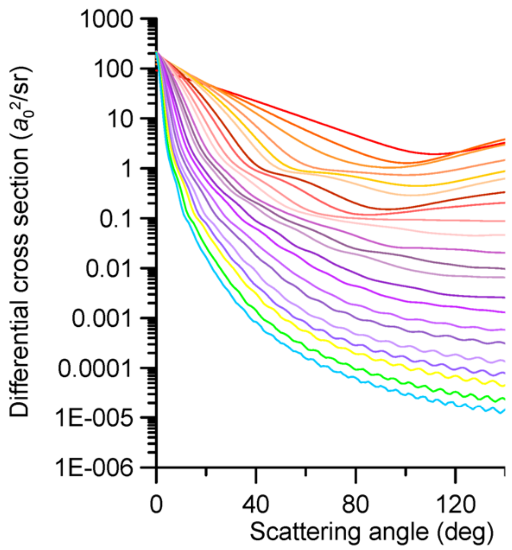
The apparatus has been perfectly set-up and all the parameters related to extraction, focusing and electron detections have been carefully optimized, with a special attention to the several voltages that are needed throughout the electron gun and chamber system. On the other hand, and due to the low energy regime that we are particular interest6ed to look at, a slightly simple system to work in electron energy ranges was also assembled. This system is composed of a tungsten filament that acts as an electron source followed by a hemispherical analyzer used to monochromatize the incoming electrons as far as their energy spread is concerned. Typically, a tungsten filament coupled with a simple extraction plate is capable of delivering low energy electrons (~5 eV) with an energy spread of around 0.5 eV due to the voltage drop across the filament electrodes. The hemispherical analyzer operates on a separate chamber.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

On the light of the recent electron scattering cross sections and stopping powers in water molecules [1], similar experiments have been performed for THF in an electron energy range of 50-5000 eV's. The total scattering cross sections have shown an uncertainty of

about 5%. Further to the optical potential method assuming an independent atom representation [2], integral elastic and inelastic cross sections have been calculated in a wide energy range from 1-10000 eV's. Time Of Flight analysis coupled to this experiment regarding the charge fragments detection has allowed together with simultaneous electron measurement to derive total and partial ionization cross sections. Therefore a careful comparison with previous theoretical and experimental data, a set of recommended integral cross sectional data can provided. Furthermore the closed combination of this data with an average excitation energy obtained from the experimental energy loss spectra in dipolar conditions (high incident electron energy ~0º scattering angle), the stopping power of electrons in THF has been obtained in the 5-5000 eV's energy range.
The above description for THF will be applied to methane shortly since CH4 is considered to be a based Tissue Equivalent Material and therefore the electron scattering data to be recorded is extremely valuable following the same procedure for THF.
As an example of what we're intent on doing, below is a spectra for electron energy loss of CH4 at 40 eV of incident electron energy with different impact angles as well as calculated elastic cross sections. With these calculations we are able to change the electron intensity in the EEL spectra to an absolute value through the normalisation of the elastic peak.





FUTURE COLLABORATION WITH HOST INSTITUTION

This research programme will continue through the exchange of post-graduate students and future missions.

PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE GRANT

At least one joint publication is to be submitted shortly. Other publications will emerge during the next months as soon as we compile and analyse the relevant data recorded.